

ASYMPTOTIC BEHAVIOUR OF CUBOIDS OPTIMISING LAPLACIAN EIGENVALUES

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ABSTRACT. We prove that in dimension $n \geq 2$, within the collection of unit measure cuboids in \mathbb{R}^n (i.e. domains of the form $\prod_{i=1}^n (0, a_i)$), any sequence of minimising domains R_k^D for the Dirichlet eigenvalues λ_k converges to the unit cube as $k \rightarrow \infty$. Correspondingly we also prove that any sequence of maximising domains R_k^N for the Neumann eigenvalues μ_k within the same collection of domains converges to the unit cube as $k \rightarrow \infty$. For $n = 2$ this result was obtained by Antunes and Freitas in the case of Dirichlet eigenvalues and van den Berg, Bucur and Gittins for the Neumann eigenvalues. The Dirichlet case for $n = 3$ was recently treated by van den Berg and Gittins.

In addition we obtain stability results for the optimal eigenvalues as $k \rightarrow \infty$. We also obtain corresponding shape optimisation results for the Riesz means of eigenvalues in the same collection of cuboids. For the Dirichlet case this allows us to address the shape optimisation of the average of the first k eigenvalues.

1. INTRODUCTION

Let $\Omega \subset \mathbb{R}^n$, $n \geq 2$, be an open set with finite Lebesgue measure $|\Omega| < \infty$. Then the spectrum of the Dirichlet Laplace operator $-\Delta_\Omega^D$ acting on $L^2(\Omega)$ is discrete and the Dirichlet eigenvalues can be written in a non-decreasing sequence, repeating each eigenvalue according to its multiplicity,

$$\lambda_1(\Omega) \leq \lambda_2(\Omega) \leq \dots \leq \lambda_k(\Omega) \leq \dots,$$

with $\lambda_1(\Omega) > 0$. Moreover, the sequence accumulates only at infinity.

If in addition the boundary of Ω is Lipschitz regular, then the spectrum of the Neumann Laplace operator $-\Delta_\Omega^N$ is discrete and its eigenvalues can be written in a non-decreasing sequence, repeating each eigenvalue according to its multiplicity,

$$0 = \mu_0(\Omega) \leq \mu_1(\Omega) \leq \dots \leq \mu_k(\Omega) \leq \dots,$$

again the sequence accumulates only at infinity.

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For $k \in \mathbb{N}$ and fixed $c > 0$, the existence of sets $\Omega_k^{\mathcal{D}}$ and $\Omega_k^{\mathcal{N}}$ which realise the infimum respectively the supremum in the optimisation problems

$$\begin{aligned}\lambda_k(\Omega_k^{\mathcal{D}}) &= \inf\{\lambda_k(\Omega) : \Omega \subset \mathbb{R}^n \text{ open, } |\Omega| = c\}, \\ \mu_k(\Omega_k^{\mathcal{N}}) &= \sup\{\mu_k(\Omega) : \Omega \subset \mathbb{R}^n \text{ open and Lipschitz, } |\Omega| = c\}\end{aligned}$$

has received a great deal of attention throughout the last century.

It was shown independently by Faber [14] and Krahn [27] that the first Dirichlet eigenvalue is minimised by the ball of measure c . Furthermore, Krahn [28] proved that the disjoint union of two balls each of measure $\frac{c}{2}$ minimises λ_2 . In the Neumann case it was shown by Szegő [39] and Weinberger [40] that the ball of measure c maximises μ_1 . Girouard, Nadirashvili and Polterovich [17] proved that among all bounded, open, planar, simply-connected sets of area c , the maximum of μ_2 is realised by a sequence of sets which degenerates to the disjoint union of two discs each of area $\frac{c}{2}$.

For $k \geq 3$, it is known that a minimiser of λ_k exists in the collection of quasi-open sets, see [10, 35]. But whether these minimisers are open is currently unresolved. In general minimisers of λ_3 are not known to date, but there are some conjectures for them, for example see [20, 37]. In the plane, and with $k \geq 5$, it is known that neither a disc nor a disjoint union of discs minimises λ_k [9]. In addition, for some values of $k \geq 3$, numerical evidence suggests that minimisers of λ_k might not have any natural symmetries, see [2].

In the Neumann case the existence of a maximising set which realises the above supremum remains open to date (see, for example, [11, Subsection 7.4]).

An idea brought forward by Antunes and Freitas [3] was to consider the behaviour of minimisers of λ_k at the other end of the spectrum. That is, for a collection of sets in which a minimiser $\Omega_k^{\mathcal{D}}$ of λ_k exists for all $k \in \mathbb{N}$, to determine the limiting shape of a sequence of minimising sets $(\Omega_k^{\mathcal{D}})_k$ as $k \rightarrow \infty$. Analogously, if a maximiser $\Omega_k^{\mathcal{N}}$ of μ_k exists in some collection of sets, then one can consider the asymptotic behaviour of a sequence of maximising sets $(\Omega_k^{\mathcal{N}})_k$ as $k \rightarrow \infty$.

It was shown in [12] that the statement that $\lambda_k(\Omega_k^{\mathcal{D}})$ resp. $\mu_k(\Omega_k^{\mathcal{N}})$ is asymptotically equal to $4\pi^2(c\omega_n)^{-2/n}k^{2/n}$ as $k \rightarrow \infty$, where ω_n is the measure of the unit ball in \mathbb{R}^n , is equivalent to Pólya's conjecture: for $k \in \mathbb{N}$ and any bounded, open set $\Omega \subset \mathbb{R}^n$ of measure c ,

$$\begin{aligned}\lambda_k(\Omega) &\geq 4\pi^2(c\omega_n)^{-2/n}k^{2/n}, \\ \mu_k(\Omega) &\leq 4\pi^2(c\omega_n)^{-2/n}k^{2/n}.\end{aligned}\tag{1}$$

These inequalities were shown to hold for tiling domains by Pólya [38], see also [26]. In particular, they hold for $\Omega = \prod_{i=1}^n (0, a_i)$.

In [3], it was shown that among all planar rectangles of unit area, any sequence of minimising rectangles for λ_k converges to the unit square as $k \rightarrow \infty$. In [7] it was shown that the corresponding result holds in the Neumann case. Furthermore, the analogous result for the Dirichlet eigenvalues in three dimensions was proven in [8]. That is, among all cuboids in \mathbb{R}^3 of unit volume, any sequence of cuboids minimising λ_k converges to the unit cube as $k \rightarrow \infty$. For the Dirichlet eigenvalues, it was conjectured in [4] that the analogous result also holds in dimensions $n \geq 4$, and some support for this conjecture was

obtained there (see [4, Section 2]). Similar arguments also suggest that the corresponding result holds for the Neumann eigenvalues in dimensions $n \geq 3$ (by invoking [4, Theorem 4] instead of [4, Theorem 1]).

Let $R \subset \mathbb{R}^n$ be an n -dimensional cuboid of unit measure, that is a domain of the form $\prod_{i=1}^n (0, a_i)$ where $a_1, \dots, a_n \in \mathbb{R}$ are such that $0 < a_1 \leq \dots \leq a_n$ and $\prod_{i=1}^n a_i = 1$. For $k \in \mathbb{N}$, $\lambda_k(R)$ and $\mu_k(R)$ obey the two-term asymptotic formulae

$$\begin{aligned}\lambda_k(R) &= 4\pi\Gamma\left(\frac{n}{2} + 1\right)^{2/n} k^{2/n} + \frac{2\pi\Gamma(\frac{n}{2} + 1)^{1+1/n}}{n\Gamma(\frac{n+1}{2})} |\partial R| k^{1/n} + o(k^{1/n}), \\ \mu_k(R) &= 4\pi\Gamma\left(\frac{n}{2} + 1\right)^{2/n} k^{2/n} - \frac{2\pi\Gamma(\frac{n}{2} + 1)^{1+1/n}}{n\Gamma(\frac{n+1}{2})} |\partial R| k^{1/n} + o(k^{1/n}),\end{aligned}\tag{2}$$

as $k \rightarrow \infty$. Here, and in what follows, $|\partial R|$ denotes the perimeter of R . Corresponding two-term asymptotic formulae were conjectured by Weyl for more general domains $\Omega \subset \mathbb{R}^n$, and under certain regularity assumptions the conjecture was proven by Ivrii in [24].

Since the cube in \mathbb{R}^n has smallest perimeter in the collection of n -dimensional cuboids, (2) suggests that the cube is the limiting domain of a sequence of optimising cuboids in this collection as $k \rightarrow \infty$. However, this argument does not provide a proof as we are not considering a fixed cuboid R and then letting $k \rightarrow \infty$, the minimising or maximising cuboids themselves depend upon k (see, for instance, [4]).

For a cuboid R as above, the Laplacian eigenvalues are given by

$$\frac{\pi^2 i_1^2}{a_1^2} + \frac{\pi^2 i_2^2}{a_2^2} + \dots + \frac{\pi^2 i_n^2}{a_n^2},\tag{3}$$

where i_1, \dots, i_n are non-negative integers in the Neumann case and positive integers in the Dirichlet case.

From (3) we see that a minimising cuboid of unit measure for λ_k , $k \in \mathbb{N}$, must exist. Indeed, as in [8], we consider a minimising sequence for λ_k where one side-length is blowing up. Then another side-length must be shrinking in order to preserve the measure constraint. However, this shrinking side would give rise to large eigenvalues, whilst for the n -dimensional unit cube Q we have that $\lambda_k(Q) \leq n\pi^2 k^2 < \infty$, contradicting the minimality of the sequence.

Similarly we see that a maximising cuboid of unit measure for μ_k , $k \in \mathbb{N}$, exists. As in [7], if $(R_\ell)_{\ell \in \mathbb{N}} = (R_{a_1^\ell, \dots, a_n^\ell})_{\ell \in \mathbb{N}}$ is a maximising sequence for μ_k with $a_n^\ell \rightarrow \infty$ as $\ell \rightarrow \infty$, then for sufficiently large ℓ

$$\mu_k(R_\ell) \leq \frac{\pi^2 k^2}{(a_n^\ell)^2}$$

and so $\mu_k(R_\ell) \rightarrow 0$ as $\ell \rightarrow \infty$. For the unit cube Q we have that $\mu_k(Q) > \pi^2$, contradicting the maximality of the sequence.

The quantity θ_n that we define below plays a central role in the results that follow.

Definition 1.1. For $n \geq 2$, define θ_n as any exponent such that for all $a_1, \dots, a_n \in \mathbb{R}_+$,

$$\#\{z \in \mathbb{Z}^n : a_1^2 z_1^2 + \dots + a_n^2 z_n^2 \leq t^2\} - \omega_n t^n \prod_{i=1}^n a_i = O(t^{\theta_n}), \quad \text{as } t \rightarrow \infty, \quad (4)$$

uniformly for a_i on compact subsets of \mathbb{R}_+ .

If (4) is not required to hold uniformly for different a_i , then estimates for θ_n are well-known (see, for instance, [19, 22, 23] and references therein). However, with the additional requirement of a uniform remainder term the literature is less extensive. For $n \geq 5$, $\theta_n = n - 2$ is known to hold and to be optimal [18]. As far as the authors are aware, the smallest known value, for $n < 5$, is $\theta_n = \frac{n(n-1)}{n+1}$ which is due to van der Corput [13] for $n = 2$ and Herz [21] for $n \geq 3$.

The main aim of this paper is to prove the following theorems, and thereby extend the results of [3, 8] and [7] to all dimensions.

Theorem 1.1. Let $n \geq 4$. For $k \in \mathbb{N}$, let $R_k^{\mathcal{D}} = R_{a_{1,k}^*, \dots, a_{n,k}^*}$ denote an n -dimensional cuboid which minimises λ_k , where $0 < a_{1,k}^* \leq \dots \leq a_{n,k}^*$ and $\prod_{i=1}^n a_{i,k}^* = 1$. Then, as $k \rightarrow \infty$, we have that

$$a_{n,k}^* = 1 + O(k^{(\theta_n - (n-1))/(2n)}),$$

where θ_n is as defined in (4). That is, any sequence of minimising n -dimensional cuboids $(R_k^{\mathcal{D}})_k$ for λ_k converges to the n -dimensional unit cube as $k \rightarrow \infty$.

Theorem 1.2. Let $n \geq 3$. For $k \in \mathbb{N}$, let $R_k^{\mathcal{N}} = R_{a_{1,k}^*, \dots, a_{n,k}^*}$ denote an n -dimensional cuboid which maximises μ_k , where $0 < a_{1,k}^* \leq \dots \leq a_{n,k}^*$ and $\prod_{i=1}^n a_{i,k}^* = 1$. Then, as $k \rightarrow \infty$, we have that

$$a_{n,k}^* = 1 + O(k^{(\theta_n - (n-1))/(2n)}),$$

where θ_n is as defined in (4). That is, any sequence of maximising n -dimensional cuboids $(R_k^{\mathcal{N}})_k$ for μ_k converges to the n -dimensional unit cube as $k \rightarrow \infty$.

A further interesting question is what this implies for the difference between λ_k^* and $\lambda_k(Q)$, resp. μ_k^* and $\mu_k(Q)$, where Q denotes the unit cube. By Pólya's inequalities (1), and the leading order asymptotics of $\lambda_k(Q)$, $\mu_k(Q)$, we see that $|\lambda_k(Q) - \lambda_k^*| = o(k^{2/n})$ and $|\mu_k(Q) - \mu_k^*| = o(k^{2/n})$. By a more detailed analysis, we obtain the following.

Theorem 1.3. As $k \rightarrow \infty$,

$$\begin{aligned} |\lambda_k(Q) - \lambda_k^*| &= O(k^{(\theta_n - (n-2))/n}), \\ |\mu_k(Q) - \mu_k^*| &= O(k^{(\theta_n - (n-2))/n}), \end{aligned}$$

where θ_n is as defined in (4).

Note that for $n \geq 5$ the above estimate states that the difference between the extremal eigenvalues and those of the unit cube remain bounded for all k , which we do not know to be the case for $n < 5$.

Let $r \geq 0$ and let $R = R_{a_1, \dots, a_n}$ be a cuboid in \mathbb{R}^n , with $a_1, \dots, a_n \in \mathbb{R}$ such that $0 < a_1 \leq \dots \leq a_n$ and $\prod_{i=1}^n a_i = 1$. We define

$$E(r, R) := \left\{ (x_1, \dots, x_n) \in \mathbb{R}^n : \sum_{j=1}^n \frac{x_j^2}{a_j^2} \leq \frac{r}{\pi^2} \right\}. \quad (5)$$

The set $E(r, R) \subset \mathbb{R}^n$ is an n -dimensional ellipsoid with radii $r_j = \frac{a_j r^{1/2}}{\pi}$, $j = 1, \dots, n$, and measure $|E(r, R)| = \omega_n \prod_{j=1}^n r_j = \frac{r^{n/2}}{\pi^{n/2} \Gamma(\frac{n}{2} + 1)}$.

By (3), we see that the Dirichlet eigenvalues $\lambda_1(R), \dots, \lambda_k(R)$ correspond to integer lattice points with positive coordinates that lie inside or on the ellipsoid $E(\lambda_k(R), R)$. In this setting, determining a cuboid of unit measure which minimises λ_k corresponds to determining the ellipsoid which contains k integer lattice points with positive coordinates and has minimal measure. Similarly, the Neumann eigenvalues $\mu_0(R), \mu_1(R), \dots, \mu_k(R)$ correspond to integer lattice points with non-negative coordinates that lie inside or on the ellipsoid $E(\mu_k(R), R)$. Determining a cuboid of unit measure which maximises μ_k corresponds to determining the ellipsoid of maximal measure which contains less than $k + 1$ integer lattice points with non-negative coordinates.

This observation is used to prove Theorems 1.1 and 1.2 by following the strategy of [3] (see also [7, 8]). In particular, we compare the number of lattice points that are inside or on a minimal, respectively maximal, ellipsoid to the number of lattice points that are inside or on the sphere with radius $\pi^{-1}(\lambda_k^*)^{1/2}$, respectively $\pi^{-1}(\mu_k^*)^{1/2}$, and let $k \rightarrow \infty$. To make this comparison, we use known estimates for the number of integer lattice points that are inside or on an n -dimensional ellipsoid (this explains the appearance of the quantity θ_n in the above results). However, in order to use these estimates, we must first show that for any sequence of minimising or maximising cuboids, the corresponding side-lengths are bounded independently of k . The difficulty lies in obtaining a sufficiently good upper, resp. lower, bound for the Dirichlet, resp. Neumann, counting function which, for $\lambda, \mu \geq 0$ and $R, E(r, R)$ as above, we define as

$$\begin{aligned} N^D(\lambda, R) &:= \#\{(i_1, \dots, i_n) \in \mathbb{N}^n \cap E(\lambda, R)\}, \\ N^N(\mu, R) &:= \#\{(i_1, \dots, i_n) \in (\mathbb{N} \cup \{0\})^n \cap E(\mu, R)\}. \end{aligned} \quad (6)$$

The approach used in [3, 7] and [8] makes use of the fact that the functions $i \mapsto (y - i^2)^{m/2}$, for $m = 1, 2$, are concave on $[0, y^{1/2}]$. However, for $m \geq 3$, this concavity fails and hence this approach cannot be used to deal with the higher-dimensional cases, see [8]. To use the same approach as in [7] to deal with the case $n = 3$, it would also be necessary to show that $\limsup_{k \rightarrow \infty} (a_{1,k}^*)^{-1} (\mu_k^*)^{-1/2} < \infty$, where $a_{1,k}^*$ is the shortest side of a cuboid maximising μ_k (compare with [7, Lemma 2.3]). The approach taken for the Neumann case here allows us to obtain a two-term lower bound for $N^N(\mu, R)$ which enables us to avoid such considerations. Nonetheless, in any dimension it is possible to obtain a bound for the quantity $\limsup_{k \rightarrow \infty} (a_{1,k}^*)^{-1} (\mu_k^*)^{-1/2}$ by exploiting that either $a_{1,k}^*$ is large or all $\mu_l(R_k^N)$,

for $l < k$, must be of the form $\pi^2 \sum_{j=2}^n i_j^2 (a_{j,k}^*)^{-2}$ and by the maximality of μ_k^* the domain $\prod_{j=2}^n (0, a_{j,k}^*)$ must be a maximiser of μ_k amongst cuboids in \mathbb{R}^{n-1} of measure $1/a_{1,k}^*$.

In this paper, in order to obtain a sufficiently sharp upper bound for $N^{\mathcal{D}}(\lambda, R)$ and corresponding lower bound for $N^{\mathcal{N}}(\mu, R)$, we make use of an argument going back to Laptev [29] and the fact that cuboids satisfy Pólya's inequalities (1). This argument allows us to reduce the problem to proving one-dimensional estimates.

Our approach naturally lifts to considering shape optimisation problems of maximising, resp. minimising, the Riesz means of Dirichlet, resp. Neumann, eigenvalues, which for $\lambda, \mu \geq 0$ and $\gamma \geq 0$ are defined by

$$\mathrm{Tr}(-\Delta_{\Omega}^{\mathcal{D}} - \lambda)_{-}^{\gamma} = \sum_{k=1}^{\infty} (\lambda - \lambda_k(\Omega))_{+}^{\gamma}, \quad \text{and} \quad \mathrm{Tr}(-\Delta_{\Omega}^{\mathcal{N}} - \mu)_{-}^{\gamma} = \sum_{k=0}^{\infty} (\mu - \mu_k(\Omega))_{+}^{\gamma}.$$

For $\Omega \subset \mathbb{R}^n$ and $\gamma \geq 3/2$ the Dirichlet case of this problem was addressed in [32], where it was shown that amongst collections of convex sets of unit measure satisfying certain additional regularity assumptions, the extremal sets converge to the ball as $\lambda \rightarrow \infty$. Within the collection of n -dimensional cuboids we obtain the corresponding result for all $\gamma \geq 0$ in both the Dirichlet and Neumann cases, that is any sequence of optimal cuboids converges to the unit cube as $\lambda, \mu \rightarrow \infty$.

A problem closely related to that considered here was recently studied by Laugesen and Liu [33]. In this article the authors consider a collection of concave, planar curves that lie in the first quadrant and have intercepts $(L, 0)$ and $(0, M)$. They fix such a curve and scale it in the x direction by s^{-1} and in the y direction by s , as well as radially by r . Their goal is to determine the curve which contains the most integer lattice points in the first quadrant as $r \rightarrow \infty$. Under certain assumptions on the curve they prove that the optimal stretch factor $s(r) \rightarrow 1$ as $r \rightarrow \infty$. In particular, they recover the result of Antunes and Freitas [3], and, in a similar way, that of van den Berg, Bucur and Gittins [7]. They also obtain analogous results for p -ellipses where $1 < p < \infty$. The case where $p = 1$ remains open. The case where $0 < p < 1$ has recently been addressed by Ariturk and Laugesen in [4]. As mentioned above, the results of that paper lend some support to Theorem 1.1 in the case where $n \geq 5$ (see [4, Section 2]).

The plan for the remainder of the paper is as follows. In Section 2.1 we obtain bounds for the eigenvalue counting functions $N^{\mathcal{D}}, N^{\mathcal{N}}$. We continue in Section 2.2 by applying the obtained bounds to prove that the side-lengths of a sequence of minimising, respectively maximising, cuboids $(R_k^{\mathcal{D}})_k, (R_k^{\mathcal{N}})_k$ are bounded independently of k . In Section 2.3 we prove uniform asymptotic expansions for the counting functions $N^{\mathcal{D}}(\lambda, R_k^{\mathcal{D}}), N^{\mathcal{N}}(\mu, R_k^{\mathcal{N}})$. All the above is combined in Section 3 in order to prove Theorems 1.1, 1.2 and 1.3. Finally, in Section 4 we apply our methods to the shape optimisation problems of maximising, resp. minimising, the Riesz means of Dirichlet, resp. Neumann, eigenvalues and minimising the average of the first k Dirichlet eigenvalues. For both problems we obtain analogous results to those obtained in the case of individual eigenvalues.

2. PRELIMINARIES

We begin this section by establishing two- respectively three-term bounds for the eigenvalue counting functions for the Neumann and Dirichlet Laplacians on an arbitrary cuboid. These bounds will allow us to prove that the sequence of extremal cuboids remains uniformly bounded, i.e. does not degenerate, as k tends to infinity, see Section 2.2.

We end this section by establishing precise and uniform asymptotics for the eigenvalue counting functions on the sequence of extremal cuboids.

Here and in what follows we let $L_{\gamma,m}^{\text{cl}}$ denote the semi-classical Lieb–Thirring constant

$$L_{\gamma,m}^{\text{cl}} = \frac{\Gamma(\gamma+1)}{(4\pi)^{m/2} \Gamma(\gamma + \frac{m}{2} + 1)}.$$

For $x \in \mathbb{R}$ we also define the positive and negative parts of x by $x_{\pm} = (|x| \pm x)/2$.

2.1. Asymptotically sharp bounds for the eigenvalue counting functions. In this section we prove a three-term upper bound for the counting function $N^{\mathcal{D}}(\lambda, R)$ and a two-term lower bound for the counting function $N^{\mathcal{N}}(\mu, R)$. More specifically we prove the following lemmas.

Lemma 2.1. *Let $R = \prod_{i=1}^n (0, a_i)$, $n \geq 4$, be such that $0 < a_1 \leq \dots \leq a_n$ and $|R| = 1$. Then the bound*

$$N^{\mathcal{D}}(\lambda, R) \leq L_{0,n}^{\text{cl}} \lambda^{n/2} - \frac{3bL_{0,n-1}^{\text{cl}}}{8a_1} \lambda^{(n-1)/2} + \frac{b^2 L_{0,n-2}^{\text{cl}}}{8\pi a_1^2} \lambda^{(n-2)/2},$$

holds for all $\lambda \geq 0$ and all $b \in [0, b_0]$, with $b_0 := \pi - \sqrt{\frac{6-8\pi+3\pi^2}{3}}$.

Lemma 2.2. *Let $R = \prod_{i=1}^n (0, a_i)$, $n \geq 2$, be such that $0 < a_1 \leq \dots \leq a_n$ and $|R| = 1$. Then, for $\mu \geq 0$,*

$$N^{\mathcal{N}}(\mu, R) \geq L_{0,n}^{\text{cl}} \mu^{n/2} + \left(1 - \frac{\pi}{4}\right) \frac{L_{0,n-1}^{\text{cl}}}{a_1} \mu^{(n-1)/2}.$$

It is not difficult to check that the three-term bounds obtained for the corresponding Dirichlet counting functions in [3, Lemma 3.1] respectively [8, Lemma 4.1] are strong enough to imply similar bounds in the cases where $n = 2, 3$. An important observation in proving such a bound is that it holds trivially for all $\lambda < \pi^2/a_1^2$.

Proposition 2.3. *Let $R = \prod_{i=1}^n (0, a_i)$, $n \in \{2, 3\}$, be such that $0 < a_1 \leq \dots \leq a_n$ and $|R| = \prod_{i=1}^n a_i = 1$. Then the bound*

$$N^{\mathcal{D}}(\lambda, R) \leq L_{0,n}^{\text{cl}} \lambda^{n/2} - \frac{3bL_{0,n-1}^{\text{cl}}}{8a_1} \lambda^{(n-1)/2} + \frac{b^2 L_{0,n-2}^{\text{cl}}}{4\pi a_1^2} \lambda^{(n-2)/2},$$

holds for all $\lambda \geq 0$ and all $b \in [0, b_0]$, with $b_0 := \frac{3\pi}{4} - \frac{1}{12} \sqrt{\pi(81\pi + 64\sqrt{6} - 288)}$.

Remark 2.4. The parameter b in our bounds for $N^{\mathcal{D}}(\lambda, R)$ allows us to tune whether we wish the bound to be more accurate near the bottom of the spectrum or asymptotically

as $\lambda \rightarrow \infty$. This flexibility will be of central importance for us when we prove the uniform boundedness of the extremal cuboids for the Dirichlet problem, see Section 2.2.

Remark 2.5. For $n \geq 5$ a bound similar to Lemma 2.1 was obtained in [31, Corollary 1.2], but without the third term and a smaller coefficient in the second one. The proof given here is, in some sense, a refinement of the method used in that paper in the special case of cuboids.

Proof of Lemmas 2.1 and 2.2. Following an idea due to Laptev [29], using the fact that cuboids satisfy Pólya's inequalities (1) and the product structure of the domain, allows us to reduce the problem to one-dimensional estimates.

To this end we let $R' = (0, a_2) \times \cdots \times (0, a_n)$ and write

$$\begin{aligned} N^{\mathcal{D}}(\lambda, R) &= \sum_{k: \lambda_k(R) \leq \lambda} (\lambda - \lambda_k(R))^0 \\ &= \sum_{k, l: \lambda_k(R') + \lambda_l((0, a_1)) \leq \lambda} (\lambda - \lambda_l((0, a_1)) - \lambda_k(R'))^0 \\ &= \sum_{l: \lambda_l((0, a_1)) \leq \lambda} \sum_{k: \lambda_k(R') \leq \lambda - \lambda_l((0, a_1))} ((\lambda - \lambda_l((0, a_1))) - \lambda_k(R'))^0 \\ &= \sum_{l: \lambda_l((0, a_1)) \leq \lambda} N^{\mathcal{D}}((\lambda - \lambda_l((0, a_1)))_+, R'), \end{aligned}$$

where we use the convention " $0^0 = 1$ ". The above could be done with strict inequalities to avoid this issue, but to match (5), (6) we also wish to count the eigenvalues that are equal to λ . Applying Pólya's inequality for the counting function on R' in the sum, $N^{\mathcal{D}}(\lambda, R') \leq L_{0, n-1}^{\text{cl}} |R'| \lambda^{(n-1)/2}$ (see [38]), yields that

$$\begin{aligned} N^{\mathcal{D}}(\lambda, R) &\leq \sum_{l: \lambda_l((0, a_1)) \leq \lambda} L_{0, n-1}^{\text{cl}} |R'| (\lambda - \lambda_l((0, a_1)))_+^{(n-1)/2} \\ &= L_{0, n-1}^{\text{cl}} |R'| \text{Tr}(-\Delta_{(0, a_1)}^{\mathcal{D}} - \lambda)_-^{(n-1)/2}. \end{aligned} \quad (7)$$

Analogously, with the only difference being that Pólya's inequality goes in the opposite direction, one finds that

$$N^{\mathcal{N}}(\mu, R) \geq L_{0, n-1}^{\text{cl}} |R'| \text{Tr}(-\Delta_{(0, a_1)}^{\mathcal{N}} - \mu)_-^{(n-1)/2}. \quad (8)$$

The Aizenman–Lieb Identity [1] asserts that if $\gamma_1 \geq 0$ and $\gamma_2 > \gamma_1$, then, for $\eta \geq 0$,

$$\text{Tr}(-\Delta_{\Omega} - \eta)_-^{\gamma_2} = B(1 + \gamma_1, \gamma_2 - \gamma_1)^{-1} \int_0^{\infty} \tau^{-1 + \gamma_2 - \gamma_1} \text{Tr}(-\Delta_{\Omega} - (\eta - \tau))_-^{\gamma_1} d\tau,$$

where B denotes the Euler Beta function, we emphasise that this is an identity for the functions $(\eta - \cdot)_+^{\gamma_i}$, with $i = 1, 2$, and thus holds equally well for any choice of boundary conditions.

Thus we can write the bounds (7) and (8) in the form

$$N^{\mathcal{D}}(\lambda, R) \leq \frac{L_{0,n-1}^{\text{cl}} |R'|}{B(1 + \gamma, \frac{n-1}{2} - \gamma)} \int_0^\lambda \tau^{-1+(n-1)/2-\gamma} \text{Tr}(-\Delta_{(0,a_1)}^{\mathcal{D}} - (\lambda - \tau))_-^\gamma d\tau, \quad (9)$$

$$N^{\mathcal{N}}(\mu, R) \geq \frac{L_{0,n-1}^{\text{cl}} |R'|}{B(1 + \gamma, \frac{n-1}{2} - \gamma)} \int_0^\mu \tau^{-1+(n-1)/2-\gamma} \text{Tr}(-\Delta_{(0,a_1)}^{\mathcal{N}} - (\mu - \tau))_-^\gamma d\tau, \quad (10)$$

where we are free to choose $\gamma \in [0, (n-1)/2)$. By choosing suitable γ and appropriate one-dimensional estimates it is possible to obtain a variety of bounds for the counting functions. The bounds that we make use of here are proven in the appendix (see Lemmas A.1 and A.2). In the Dirichlet case the bound states that

$$\text{Tr}(-\Delta_{(0,a)}^{\mathcal{D}} - \lambda)_-^{3/2} \leq aL_{3/2,1}^{\text{cl}} \lambda^2 - \frac{3b}{8} L_{3/2,0}^{\text{cl}} \lambda^{3/2} + \frac{b^2}{8\pi a} L_{3/2,-1}^{\text{cl}} \lambda, \quad (11)$$

for all $\lambda \geq 0, a > 0$ and $b \in [0, b_0]$, with $b_0 := \pi - \sqrt{\frac{6-8\pi+3\pi^2}{3}}$. For the Neumann case we have instead that

$$\text{Tr}(-\Delta_{(0,a)}^{\mathcal{N}} - \mu)_-^{1/2} \geq aL_{1/2,1}^{\text{cl}} \mu + \left(1 - \frac{\pi}{4}\right) L_{1/2,0}^{\text{cl}} \sqrt{\mu}, \quad (12)$$

which is valid for all $\mu \geq 0$ and $a > 0$.

The Dirichlet case: For $n = 4$ we do not need to use the Aizenman–Lieb Identity, instead apply the bound in (11) to the one-dimensional trace of (7) which yields the claimed bound. For dimensions $n \geq 5$ choose $\gamma = 3/2$ in (9) and apply (11), computing the resulting integral completes the proof of Lemma 2.1.

The Neumann case: For $n = 2$ the bound follows from combining (8) with (12). For dimensions $n \geq 3$ choose $\gamma = 1/2$ in (10) and apply (12). Computing the resulting integral completes the proof. \square

2.2. Extremal cuboids are uniformly bounded. In this section we obtain a uniform upper bound for the longest side-length of the extremal cuboids $R_k^{\mathcal{D}}$ and $R_k^{\mathcal{N}}$.

As the proof is almost precisely the same for the Neumann and the Dirichlet cases we only write out the latter in full. The only difference between the two cases is that an element of the proof in the Dirichlet case is not present in the proof of the Neumann result. This difference stems from the fact that in the Dirichlet case we have a three-term bound and so we need to bound the quantity that this extra term gives rise to.

For $n \geq 4$ let $R^{\mathcal{D}} = R_{a_{1,k}^*, \dots, a_{n,k}^*}$ be a sequence of unit measure cuboids minimising λ_k , i.e. such that $\lambda_k(R_k^{\mathcal{D}}) = \lambda_k^*$, and assume that $a_{1,k}^* \leq \dots \leq a_{n,k}^*$. By the optimality of $R_k^{\mathcal{D}}$ we have, for any $0 < \varepsilon < 1$, that

$$N^{\mathcal{D}}(\lambda_k^* - \varepsilon, Q) \leq N^{\mathcal{D}}(\lambda_k^*, R_k^{\mathcal{D}}),$$

where as before Q denotes the n -dimensional unit cube.

The two-term asymptotics for the Dirichlet eigenvalue counting function on the cube (see [24] or Section 2.3) combined with Lemma 2.1 then yields that

$$\begin{aligned} L_{0,n}^{\text{cl}}(\lambda_k^* - \varepsilon)^{n/2} - \frac{L_{0,n-1}^{\text{cl}}}{4} |\partial Q| (\lambda_k^* - \varepsilon)^{(n-1)/2} + o((\lambda_k^* - \varepsilon)^{(n-1)/2}) \\ \leq L_{0,n}^{\text{cl}}(\lambda_k^*)^{n/2} - \frac{3bL_{0,n-1}^{\text{cl}}}{8a_{1,k}^*} (\lambda_k^*)^{(n-1)/2} + \frac{b^2L_{0,n-2}^{\text{cl}}}{8\pi(a_{1,k}^*)^2} (\lambda_k^*)^{n/2-1}. \end{aligned}$$

Rearranging and taking $\varepsilon = O(1)$ we find that

$$\frac{b}{a_{1,k}^*} \left(1 - \frac{bL_{0,n-2}^{\text{cl}}(\lambda_k^*)^{-1/2}}{3\pi L_{0,n-1}^{\text{cl}}a_{1,k}^*} \right) \leq \frac{4n}{3} + o(1).$$

Since $\lambda_k^* = \lambda_k(R_k^{\mathcal{D}}) \geq \lambda_1(R_k^{\mathcal{D}}) > \pi^2(a_{1,k}^*)^{-2}$, we have that $-(\lambda_k^*)^{-1/2} \geq -a_{1,k}^*/\pi$. Hence

$$\frac{b}{a_{1,k}^*} \left(1 - \frac{bL_{0,n-2}^{\text{cl}}}{3\pi^2 L_{0,n-1}^{\text{cl}}} \right) \leq \frac{4n}{3} + o(1).$$

We now choose $b \in (0, b_0]$, where b_0 is as defined in Lemma 2.1, to maximise the left-hand side (note that the maximum is in fact positive). This amounts to choosing $b = \min\left\{b_0, \frac{3\pi^2 L_{0,n-1}^{\text{cl}}}{2L_{0,n-2}^{\text{cl}}}\right\}$, if $n \leq 22$ the first option is minimal while for higher dimensions we choose the second.

Let $M(n)$ be defined by

$$\begin{aligned} M(n) &:= \sup \left\{ b - \frac{b^2 L_{0,n-2}^{\text{cl}}}{3\pi^2 L_{0,n-1}^{\text{cl}}} : b \in (0, b_0] \right\} \\ &= \begin{cases} \frac{3\pi - \sqrt{3(6-8\pi+3\pi^2)}}{27\pi^{3/2}\Gamma(\frac{n}{2})} (9\pi^{3/2}\Gamma(\frac{n}{2}) + 2(\sqrt{3(6-8\pi+3\pi^2)} - 3\pi)\Gamma(\frac{n+1}{2})), & \text{if } n \leq 22, \\ \frac{3\pi^{3/2}\Gamma(\frac{n}{2})}{8\Gamma(\frac{n+1}{2})}, & \text{if } n > 22, \end{cases} \\ &\geq \frac{\pi^{3/2}\Gamma(\frac{n}{2})}{8\Gamma(\frac{n+1}{2})^2}, \end{aligned}$$

where the last inequality is trivial if $n > 22$ and can be checked for the remaining cases $4 \leq n \leq 22$ via computer.

Then the above implies that

$$\frac{1}{a_{1,k}^*} \leq \frac{4n}{3M(n)} + o(1) \leq \frac{32n\Gamma(\frac{n+1}{2})^2}{3\pi^{3/2}\Gamma(\frac{n}{2})} + o(1), \quad (13)$$

which implies that

$$a_{n,k}^* \leq \left(\frac{1}{a_{1,k}^*} \right)^{n-1} \leq \left(\frac{32n\Gamma(\frac{n+1}{2})^2}{3\pi^{3/2}\Gamma(\frac{n}{2})} \right)^{n-1} + o(1).$$

Thus $\limsup_{k \rightarrow \infty} a_{n,k}^* < \infty$ so the side-lengths of a minimising sequence of cuboids are uniformly bounded. For dimensions $n = 2, 3$, the corresponding result was obtained, through a slightly different argument, in [3, 8] but follows by the same argument as above using Proposition 2.3. In addition, by invoking the same method as in the proof of Lemma 4.2 in [8], it is possible to obtain an explicit upper bound for $a_{n,k}^*$.

To prove the corresponding result for the Neumann problem one can take the same approach: observe that $N^\mathcal{N}(\mu_k^* - \varepsilon, R_k^\mathcal{N}) \leq N^\mathcal{N}(\mu_k^*, Q)$, for $k \geq 1$ and any $0 < \varepsilon < 1$, apply the lower bound of Lemma 2.2 to the left-hand side and expand the right-hand side using its two-term asymptotic expansion. Rearranging the obtained inequality yields a bound of the form (13).

2.3. Precise asymptotics for eigenvalue counting functions. Let $\lambda, \mu, r \geq 0$ and $E(r, R)$, $N^\mathcal{D}(\lambda, R)$ and $N^\mathcal{N}(\mu, R)$ be as defined in Section 1. Assume that $R = R_{a_1, \dots, a_n}$ has bounded side-lengths so that the ellipsoid $E(r, R)$ has strictly positive Gaussian curvature. In this section, we study the two-term asymptotic expansion of $N^\mathcal{D}(\lambda, R)$ and $N^\mathcal{N}(\mu, R)$ with remainder estimates which are uniform in the side-lengths of R . As the calculations for the Dirichlet and Neumann problems are almost identical, we will write out the argument in full only for the Dirichlet case and indicate what differences appear for the Neumann case.

For domains $\Omega \subset \mathbb{R}^n$ satisfying certain geometric conditions (see, for example, [24]), the Dirichlet and Neumann counting functions have the following two-term asymptotic expansions:

$$\begin{aligned} N^\mathcal{D}(\lambda, \Omega) &:= \#\{\lambda_k(\Omega) \leq \lambda\} = L_{0,n}^{\text{cl}} |\Omega| \lambda^{n/2} - \frac{L_{0,n-1}^{\text{cl}}}{4} |\partial\Omega| \lambda^{(n-1)/2} + o(\lambda^{(n-1)/2}), \\ N^\mathcal{N}(\mu, \Omega) &:= \#\{\mu_k(\Omega) \leq \mu\} = L_{0,n}^{\text{cl}} |\Omega| \mu^{n/2} + \frac{L_{0,n-1}^{\text{cl}}}{4} |\partial\Omega| \mu^{(n-1)/2} + o(\mu^{(n-1)/2}), \end{aligned}$$

as $\lambda, \mu \rightarrow \infty$. More generally, for the Riesz means of order $\gamma \geq 0$, we have that

$$\begin{aligned} \text{Tr}(-\Delta_\Omega^\mathcal{D} - \lambda)_-^\gamma &= L_{\gamma,n}^{\text{cl}} |\Omega| \lambda^{\gamma+n/2} - \frac{L_{\gamma,n-1}^{\text{cl}}}{4} |\partial\Omega| \lambda^{\gamma+(n-1)/2} + o(\lambda^{\gamma+(n-1)/2}), \\ \text{Tr}(-\Delta_\Omega^\mathcal{N} - \mu)_-^\gamma &= L_{\gamma,n}^{\text{cl}} |\Omega| \mu^{\gamma+n/2} + \frac{L_{\gamma,n-1}^{\text{cl}}}{4} |\partial\Omega| \mu^{\gamma+(n-1)/2} + o(\mu^{\gamma+(n-1)/2}), \end{aligned}$$

as $\lambda, \mu \rightarrow \infty$.

For notational simplicity, in what follows we will write $N^\mathcal{D}(\lambda)$, $N^\mathcal{N}(\mu)$ and $E(r)$ with the dependence on R being implicit.

Let

$$T(r) = \#\{(x_1, \dots, x_n) \in \mathbb{Z}^n \cap E(r)\}$$

be the total number of integer lattice points that are inside or on the ellipsoid $E(r)$. Furthermore, for $2 \leq m \leq n-1$, we define

$$T_{1,\dots,n-m}(r) = \#\{(0, \dots, 0, x_{n-m+1}, \dots, x_n) \in \mathbb{Z}^n \cap E(r)\},$$

and

$$T_{1,\dots,n-m}^+(r) = \#\{(0, \dots, 0, x_{n-m+1}, \dots, x_n) \in \mathbb{N}^n \cap E(r)\}.$$

Similarly, we define $T_{i_1,\dots,i_{n-m}}(r)$, $T_{i_1,\dots,i_{n-m}}^+(r)$ for $i_1, \dots, i_{n-m} \in \{1, 2, \dots, n\}$, $i_j \neq i_\ell$ for $j \neq \ell$.

For $2 \leq m \leq n-1$, $T_{1,\dots,n-m}(r)$ is the number of integer lattice points that are inside or on the m -dimensional ellipsoid which is centred at the origin and has radii $\frac{a_{n-m+1}r^{1/2}}{\pi}, \frac{a_{n-m+2}r^{1/2}}{\pi}, \dots, \frac{a_n r^{1/2}}{\pi}$. In particular, if $m = 2$, then $T_{1,\dots,n-2}(r)$ is an ellipse which is centred at the origin and has radii $\frac{a_{n-1}r^{1/2}}{\pi}, \frac{a_n r^{1/2}}{\pi}$.

With this notation, we have that

$$\begin{aligned} T(\lambda) &= 2^n N^{\mathcal{D}}(\lambda) + \sum_{k=1}^{n-2} \frac{2^{n-k}}{k!} \sum_{j_1=1}^n \sum_{j_2=1, j_2 \neq j_1}^n \cdots \sum_{j_k=1, j_k \neq j_1, \dots, j_{k-1}}^n T_{j_1, \dots, j_k}^+(\lambda) \\ &\quad + 2 \sum_{j=1}^n \left\lfloor \frac{a_j \lambda^{1/2}}{\pi} \right\rfloor + 1, \end{aligned}$$

and similarly

$$\begin{aligned} T(\mu) &= 2^n N^{\mathcal{N}}(\mu) - \sum_{k=1}^{n-2} \frac{2^{n-k}}{k!} \sum_{j_1=1}^n \sum_{j_2=1, j_2 \neq j_1}^n \cdots \sum_{j_k=1, j_k \neq j_1, \dots, j_{k-1}}^n T_{j_1, \dots, j_k}^+(\mu) \\ &\quad - 2(2^n - 1) \sum_{j=1}^n \left\lfloor \frac{a_j \mu^{1/2}}{\pi} \right\rfloor - (2^n - 1). \end{aligned}$$

Rearranging we find that

$$\begin{aligned} N^{\mathcal{D}}(\lambda) &= \frac{1}{2^n} T(\lambda) - \sum_{k=1}^{n-2} \frac{1}{k! \cdot 2^k} \sum_{j_1=1}^n \sum_{j_2=1, j_2 \neq j_1}^n \cdots \sum_{j_k=1, j_k \neq j_1, \dots, j_{k-1}}^n T_{j_1, \dots, j_k}^+(\lambda) \\ &\quad - \frac{1}{2^{n-1}} \sum_{j=1}^n \left\lfloor \frac{a_j \lambda^{1/2}}{\pi} \right\rfloor - \frac{1}{2^n}, \tag{14} \\ N^{\mathcal{N}}(\mu) &= \frac{1}{2^n} T(\mu) + \sum_{k=1}^{n-2} \frac{1}{k! \cdot 2^k} \sum_{j_1=1}^n \sum_{j_2=1, j_2 \neq j_1}^n \cdots \sum_{j_k=1, j_k \neq j_1, \dots, j_{k-1}}^n T_{j_1, \dots, j_k}^+(\mu) \\ &\quad + \frac{(2^n - 1)}{2^{n-1}} \sum_{j=1}^n \left\lfloor \frac{a_j \mu^{1/2}}{\pi} \right\rfloor + \frac{(2^n - 1)}{2^n}. \end{aligned}$$

Let $p \in \{1, \dots, n-2\}$ and fix $j_1, \dots, j_p \in \{1, \dots, n\}$ such that $j_i \neq j_\ell$ for $i \neq \ell$. Then, similarly to the above, we have that

$$\begin{aligned} T_{j_1, \dots, j_p}^+(r) &= \frac{1}{2^{n-p}} T_{j_1, \dots, j_p}(r) \\ &\quad - \sum_{k=1}^{n-2-p} \frac{1}{k! \cdot 2^k} \sum_{j_{p+1}=1, j_{p+1} \neq j_1, \dots, j_p}^n \cdots \sum_{j_{p+k}=1, j_{p+k} \neq j_1, \dots, j_{p+k-1}}^n T_{j_1, \dots, j_{p+k}}^+(r) \\ &\quad - \frac{1}{2^{n-1-p}} \sum_{j=1, j \neq j_1, \dots, j_p}^n \left\lfloor \frac{a_j r^{1/2}}{\pi} \right\rfloor - \frac{1}{2^{n-p}}. \end{aligned} \quad (15)$$

By substituting (15) with $p = 1$ into (14), we obtain that

$$\begin{aligned} N^D(\lambda) &= \frac{1}{2^n} T(\lambda) - \frac{1}{2^n} \sum_{j_1=1}^n T_{j_1}(\lambda) + \frac{1}{2 \cdot 2^2} \sum_{j_1=1}^n \sum_{j_2=1, j_2 \neq j_1}^n T_{j_1, j_2}^+(\lambda) \\ &\quad + \sum_{k=3}^{n-2} \frac{k-1}{2^k k!} \sum_{j_1=1}^n \sum_{j_2=1, j_2 \neq j_1}^n \cdots \sum_{j_k=1, j_k \neq j_1, \dots, j_{k-1}}^n T_{j_1, \dots, j_k}^+(\lambda) \\ &\quad + \frac{(n-2)}{2^{n-1}} \sum_{j=1}^n \left\lfloor \frac{a_j \lambda^{1/2}}{\pi} \right\rfloor + \frac{(n-1)}{2^n}. \end{aligned} \quad (16)$$

Again substituting (15) with $p = 2$ into (16), yields

$$\begin{aligned} N^D(\lambda) &= \frac{1}{2^n} T(\lambda) - \frac{1}{2^n} \sum_{j_1=1}^n T_{j_1}(\lambda) + \frac{1}{2 \cdot 2^n} \sum_{j_1=1}^n \sum_{j_2=1, j_2 \neq j_1}^n T_{j_1, j_2}(\lambda) \\ &\quad - \sum_{k=3}^{n-2} \frac{(k-1)(k-2)}{2^{k+1} k!} \sum_{j_1=1}^n \cdots \sum_{j_k=1, j_k \neq j_1, \dots, j_{k-1}}^n T_{j_1, \dots, j_k}^+(\lambda) \\ &\quad + \left((n-2) - \binom{n-1}{2} \right) \frac{1}{2^{n-1}} \sum_{j=1}^n \left\lfloor \frac{a_j \lambda^{1/2}}{\pi} \right\rfloor + \left((n-1) - \binom{n}{2} \right) \frac{1}{2^n}. \end{aligned} \quad (17)$$

Analogously one finds a similar expression for the Neumann counting function

$$\begin{aligned} N^N(\mu) &= \frac{1}{2^n} T(\mu) + \frac{1}{2^n} \sum_{j_1=1}^n T_{j_1}(\mu) - \frac{1}{2 \cdot 2^n} \sum_{j_1=1}^n \sum_{j_2=1, j_2 \neq j_1}^n T_{j_1, j_2}(\mu) \\ &\quad + \sum_{k=3}^{n-2} \frac{(k-1)(k-2)}{2^{k+1} k!} \sum_{j_1=1}^n \cdots \sum_{j_k=1, j_k \neq j_1, \dots, j_{k-1}}^n T_{j_1, \dots, j_k}^+(\mu) \\ &\quad + \left(2^n - n + \binom{n-1}{2} \right) \frac{1}{2^{n-1}} \sum_{j=1}^n \left\lfloor \frac{a_j \mu^{1/2}}{\pi} \right\rfloor + \left(2^n - n - 1 + \binom{n}{2} \right) \frac{1}{2^n}. \end{aligned} \quad (18)$$

By the definition of θ_n (see (4)) we have that, for $a_1, \dots, a_n > 0$,

$$\begin{aligned} T(r) &= \frac{\omega_n r^{n/2}}{\pi^n} \prod_{i=1}^n a_i + O(r^{\theta_n/2}), \\ T_{1,\dots,n-m}(r) &= \frac{\omega_m r^{m/2}}{\pi^m} \prod_{i=n-m}^n a_i + O(r^{\theta_m/2}), \\ T_{1,\dots,n-m}^+(r) &= \frac{\omega_m r^{m/2}}{2^m \pi^m} \prod_{i=n-m}^n a_i + O(r^{\theta_m/2}). \end{aligned}$$

Similar estimates also hold for the quantities $T_{j_1,\dots,j_p}(r)$ and $T_{j_1,\dots,j_p}^+(r)$, where $j_1, \dots, j_p \in \{1, \dots, n\}$ with $j_i \neq j_\ell$ for $i \neq \ell$. Note that the parameter r here is the square of the parameter usually appearing in these bounds (c.f. Definition 1.1), and moreover that the error terms are uniform for any family of ellipsoids such that a_1, \dots, a_n are uniformly bounded from above and away from zero.

By combining (17) and (18) with the above estimates, and noting that $\theta_n \in [n-2, n-1]$, we obtain the following lemma.

Lemma 2.6. *For $n \geq 2$ and $R = \prod_{i=1}^n (0, a_i) \subset \mathbb{R}^n$, with $a_i > 0$,*

$$N^{\mathcal{D}}(\lambda, R) = L_{0,n}^{cl} |R| \lambda^{n/2} - \frac{L_{0,n-1}^{cl}}{4} |\partial R| \lambda^{(n-1)/2} + O(\lambda^{\theta_n/2}), \quad (19)$$

$$N^{\mathcal{N}}(\mu, R) = L_{0,n}^{cl} |R| \mu^{n/2} + \frac{L_{0,n-1}^{cl}}{4} |\partial R| \mu^{(n-1)/2} + O(\mu^{\theta_n/2}), \quad (20)$$

as $\lambda, \mu \rightarrow \infty$, where θ_n is as defined in (4). Moreover, the remainder terms are uniform on any collection of cuboids with side-lengths contained in a compact subset of \mathbb{R}_+ .

3. GEOMETRIC CONVERGENCE & SPECTRAL STABILITY

In this section, we prove Theorems 1.1, 1.2 and 1.3. As the proofs of the Dirichlet and the Neumann cases are almost identical we again write out the former case in full and indicate the differences which occur in the proof of the latter.

Since the minimisers $R_k^{\mathcal{D}}$, respectively the maximisers $R_k^{\mathcal{N}}$, need not be unique, we consider an arbitrary subsequence of such extremal sets. By the results obtained in Section 2.2 (or the corresponding statements in [3, 8] and [7]), we know that the extremal cuboids in any dimension are uniformly bounded in k , and thus the remainder terms in (19) and (20) are uniform with respect to $R_k^{\mathcal{D}}$ and $R_k^{\mathcal{N}}$, respectively.

Proof of Theorems 1.1 and 1.2. Let as before $R_k^{\mathcal{D}} = R_{a_{1,k}^*, \dots, a_{n,k}^*}$, with $a_{1,k}^* \leq \dots \leq a_{n,k}^*$, and let Q denote the n -dimensional unit cube. Since $\lambda_k(Q) \geq \lambda_k^*$ we have, for any $0 < \varepsilon < 1$, that $N(\lambda_k^* - \varepsilon, Q) < k \leq N(\lambda_k^*, R_k^{\mathcal{D}})$. Plugging in the asymptotic expansion (19) on both

sides, we have that

$$\begin{aligned} L_{0,n}^{\text{cl}}(\lambda_k^* - \varepsilon)^{n/2} - \frac{L_{0,n-1}^{\text{cl}}}{4} |\partial Q| (\lambda_k^* - \varepsilon)^{(n-1)/2} - O((\lambda_k^* - \varepsilon)^{\theta_n/2}) \\ \leq L_{0,n}^{\text{cl}}(\lambda_k^*)^{n/2} - \frac{L_{0,n-1}^{\text{cl}}}{4} |\partial R_k^{\mathcal{D}}| (\lambda_k^*)^{(n-1)/2} + O((\lambda_k^*)^{\theta_n/2}). \end{aligned}$$

Rearranging and choosing $\varepsilon = O(1)$, we obtain that

$$|\partial R_k^{\mathcal{D}}| - |\partial Q| \leq O((\lambda_k^*)^{(\theta_n - (n-1))/2}) = O(k^{(\theta_n - (n-1))/n}), \quad (21)$$

which, when combined with the isoperimetric inequality for cuboids, implies that

$$|\partial R_k^{\mathcal{D}}| = \sum_{i=1}^n \frac{2}{a_{i,k}^*} = 2n + O(k^{(\theta_n - (n-1))/n}). \quad (22)$$

By the arithmetic – geometric means inequality, with $a_{n,k}^* = 1 + \delta_k > 1$, we find that

$$(n-1)(1 + \delta_k)^{1/(n-1)} + \frac{1}{1 + \delta_k} \leq \sum_{i=1}^n \frac{1}{a_{i,k}^*}. \quad (23)$$

Then, by (22) and (23),

$$(n-1)(1 + \delta_k)^{n/(n-1)} + 1 \leq n + n\delta_k + O(k^{(\theta_n - (n-1))/n}). \quad (24)$$

For each $n \geq 2$, we know by the results in Section 2.2 (or from [3, 8]) that there exists $T > 0$ so that $\delta_k^* = a_{n,k}^* - 1 \leq T$. Hence, letting $c(T) = \frac{(1+T)^{n/(n-1)} - 1 - \frac{n}{n-1}T}{T^2} > 0$, we have that

$$(1 + \delta_k)^{n/(n-1)} \geq 1 + \frac{n}{n-1} \delta_k + c(T) \delta_k^2.$$

By substituting this into (24), we deduce that $\delta_k = O(k^{(\theta_n - (n-1))/(2n)})$.

For the Neumann case one can argue almost identically by observing (as in the proof of the uniform boundedness of $R_k^{\mathcal{N}}$) that, for any $0 < \varepsilon < 1$,

$$N^{\mathcal{N}}(\mu_k^* - \varepsilon, R_k^{\mathcal{N}}) \leq N^{\mathcal{N}}(\mu_k^*, Q). \quad \square$$

Remark 3.1. For $n = 2, 3$, this convergence result was already proven in Section 3(d) of [3], resp. Section 5 of [8]. Similar arguments also hold for the case $n = 4$ and give rise to the above result. A difficulty in using the approach of [3, 8] is that we must control the multiplicity Θ_k of $\lambda_k(Q)$. That is

$$\Theta_k = \# \left\{ (i_1, \dots, i_n) \in \mathbb{N}^n : i_1^2 + \dots + i_n^2 = \frac{\lambda_k(Q)}{\pi^2} \right\}.$$

For $2 \leq n \leq 4$, estimates for this quantity are well known, especially in the number theory literature (for example see [23, Section 2], as well as [25, 36] and references therein). As far as the authors are aware, in general, for $n \geq 5$, estimates for the sum of squares function in terms of standard functions are not known.

Remark 3.2. We remark that if we restrict the collection of cuboids to a sub-collection, then the above arguments prove that any sequence of minimising, resp. maximising, cuboids converges to the cuboid of smallest perimeter in this sub-collection (in particular, replace Q by this cuboid in (21)). For example, in the sub-collection consisting of all cuboids in \mathbb{R}^n of the form $\prod_{i=1}^n (0, a_i)$ such that $0 < a_1 \leq \dots \leq a_n$ and $ca_1 = a_2$, with $c \geq 1$, any sequence of optimisers converges to the cuboid with $a_1 = c^{-(n-1)/n}$ and $a_2 = \dots = a_n = c^{1/n}$.

We now turn to the question of spectral stability and the proof of Theorem 1.3.

Proof of Theorem 1.3. As above let $R_k^{\mathcal{D}} = R_{a_{1,k}^*, \dots, a_{n,k}^*}$ be an arbitrary sequence of minimising cuboids, and assume that $a_{1,k}^* \leq \dots \leq a_{n,k}^*$. As in the proof of Theorems 1.1 and 1.2, we have that, for any $0 < \varepsilon < 1$, $N_k^{\mathcal{D}}(\lambda_k^* - \varepsilon, Q) \leq k \leq N_k^{\mathcal{D}}(\lambda_k^*, R_k^{\mathcal{D}})$. By the asymptotic expansion (19) we thus find that

$$\begin{aligned} L_{0,n}^{\text{cl}}(\lambda_k^* - \varepsilon)^{n/2} - \frac{L_{0,n-1}^{\text{cl}}}{4} |\partial Q| (\lambda_k^* - \varepsilon)^{(n-1)/2} - O((\lambda_k^* - \varepsilon)^{\theta_n/2}) \\ \leq k \leq L_{0,n}^{\text{cl}}(\lambda_k^*)^{n/2} - \frac{L_{0,n-1}^{\text{cl}}}{4} |\partial R_k^{\mathcal{D}}| (\lambda_k^*)^{(n-1)/2} + O((\lambda_k^*)^{\theta_n/2}). \end{aligned}$$

By the isoperimetric inequality for cuboids this also holds with $|\partial R_k^{\mathcal{D}}|$ replaced by $|\partial Q|$.

Choosing $\varepsilon = O(1)$ yields that

$$k = L_{0,n}^{\text{cl}}(\lambda_k^*)^{n/2} - \frac{L_{0,n-1}^{\text{cl}}}{4} |\partial Q| (\lambda_k^*)^{(n-1)/2} + O((\lambda_k^*)^{\theta_n/2}), \quad (25)$$

as $k \rightarrow \infty$. From which we can conclude that

$$\lambda_k^* = 4\pi\Gamma\left(\frac{n}{2} + 1\right)^{2/n} k^{2/n} + \frac{2\pi\Gamma(\frac{n}{2} + 1)^{1+1/n}}{n\Gamma(\frac{n+1}{2})} |\partial Q| k^{1/n} + O(k^{(\theta_n - (n-2))/n}), \quad (26)$$

as $k \rightarrow \infty$. Now (25) is the same two-term expansion as that for $N(\lambda, Q)$, so (26) must agree with the two-term expansion for $\lambda_k(Q)$. Thus we obtain that $|\lambda_k(Q) - \lambda_k^*| = O(k^{(\theta_n - (n-2))/n})$ as $k \rightarrow \infty$.

The approach to prove the Neumann case is identical except for that one instead uses that, for any $0 < \varepsilon < 1$,

$$N^{\mathcal{N}}(\mu_k^* - \varepsilon, R_k^{\mathcal{N}}) \leq k \leq N^{\mathcal{N}}(\mu_k^*, Q). \quad \square$$

4. RIESZ MEANS AND EIGENVALUE AVERAGES

Given the techniques and bounds above, it is not difficult to obtain the corresponding shape optimisation results for the following problems:

(1) For $\gamma \geq 0$ and $\lambda, \mu \geq 0$,

$$\begin{aligned} \sup \{ \text{Tr}(-\Delta_R^{\mathcal{D}} - \lambda)_-^\gamma : R = R_{a_1, \dots, a_n}, |R| = 1 \}, \\ \inf \{ \text{Tr}(-\Delta_R^{\mathcal{N}} - \mu)_-^\gamma : R = R_{a_1, \dots, a_n}, |R| = 1 \}. \end{aligned}$$

(2) For $k \in \mathbb{N}$,

$$\inf \left\{ \frac{1}{k} \sum_{i=1}^k \lambda_i(R) : R = R_{a_1, \dots, a_n}, |R| = 1 \right\}.$$

In a similar manner to the above (see also [32]), one can conclude that for any fixed λ, μ or $k \in \mathbb{N}$ each of these problems has at least one extremal cuboid, which we denote by $R_\lambda^{\mathcal{D}}, R_\mu^{\mathcal{N}}$ and $\bar{R}_k^{\mathcal{D}}$, respectively, where the bar is to distinguish from the minimisers of the individual eigenvalues. Problem (2) was recently treated in [15] in a more general setting, and the leading order asymptotic behaviour of the extremal eigenvalue averages was obtained.

The approach we take to solve the first problem is to use the Aizenman–Lieb Identity to lift our bounds for the counting functions to higher order Riesz means. For $\gamma \geq 1$ this improves special cases of a pair of inequalities due to Berezin [5] (see also [29]). For the second problem we use an approach based on the close relationship between the sum of eigenvalues and the Riesz means of order $\gamma = 1$. This will allow us to obtain a three-term bound for the sum of the first k eigenvalues, which improves a special case of a bound obtained by Li and Yau [34].

In the Dirichlet case we will, for notational simplicity, only treat $n \geq 4$, the corresponding results for $n = 2, 3$ follow analogously by applying Proposition 2.3 instead of using Lemma 2.1.

Lemma 4.1. *Let $\gamma \geq 0$ and let $R = R_{a_1, \dots, a_n} \subset \mathbb{R}^n$, $n \geq 4$, be such that $a_1 \leq \dots \leq a_n$ and $|R| = 1$. Then the bound*

$$\mathrm{Tr}(-\Delta_R^{\mathcal{D}} - \lambda)_-^\gamma \leq L_{\gamma, n}^{cl} \lambda^{\gamma+n/2} - \frac{3bL_{\gamma, n-1}^{cl}}{8a_1} \lambda^{\gamma+(n-1)/2} + \frac{b^2 L_{\gamma, n-2}^{cl}}{8\pi a_1^2} \lambda^{\gamma+(n-2)/2},$$

holds for all $\lambda \geq 0$ and all $b \in [0, b_0]$, with $b_0 := \pi - \sqrt{\frac{6-8\pi+3\pi^2}{3}}$.

Lemma 4.2. *Let $\gamma \geq 0$ and let $R = R_{a_1, \dots, a_n} \subset \mathbb{R}^n$, $n \geq 2$, be such that $a_1 \leq \dots \leq a_n$ and $|R| = 1$. Then the bound*

$$\mathrm{Tr}(-\Delta_R^{\mathcal{N}} - \mu)_-^\gamma \geq L_{\gamma, n}^{cl} \mu^{\gamma+n/2} + \left(1 - \frac{\pi}{4}\right) \frac{L_{\gamma, n-1}^{cl}}{a_1} \mu^{\gamma+(n-1)/2},$$

holds for all $\mu \geq 0$.

Proof of Lemmas 4.1 and 4.2. Applying the Aizenman–Lieb Identity (see [1], or Section 2.2 above) with $\gamma_1 = 0$ and $\gamma_2 = \gamma$ to both sides of Lemma 2.1, respectively Lemma 2.2, yields the result. \square

We note that by using the Laplace transform instead of the Aizenman–Lieb Identity, one could apply the above procedure to obtain a three-term bound for $\mathrm{Tr}(e^{t\Delta_R^{\mathcal{D}/\mathcal{N}}})$ valid for all cuboids $R \in \mathbb{R}^n$. Moreover, using Theorem 1.1 of [31] one can obtain a tunable three-term bound (similar to Lemma 4.1) for any convex domain $\Omega \subset \mathbb{R}^n$ which could then, using the Laplace transform, be lifted to a corresponding bound for $\mathrm{Tr}(e^{t\Delta_\Omega^{\mathcal{D}}})$. A similar inequality

was obtained by van den Berg in [6] for the Dirichlet Laplacian on smooth convex domains. By using results from [30], the upper bound of [6] can be extended to all convex domains.

Lemma 4.3. *Let $R = R_{a_1, \dots, a_n} \subset \mathbb{R}^n$, $n \geq 4$, be such that $a_1 \leq \dots \leq a_n$ and $|R| = 1$. Then the bound*

$$\frac{1}{k} \sum_{i=1}^k \lambda_i(R) \geq \frac{4\pi n \Gamma(\frac{n}{2} + 1)^{2/n}}{n+2} k^{2/n} + \frac{3\pi b \Gamma(\frac{n}{2} + 1)^{1+1/n}}{2a_1 \Gamma(\frac{n+3}{2})} k^{1/n} - \frac{b^2}{2a_1^2},$$

holds for all $k \in \mathbb{N}$ and all $b \in [0, b_0]$, with $b_0 := \pi - \sqrt{\frac{6-8\pi+3\pi^2}{3}}$.

Proof of Lemma 4.3. It is well known that the sum of eigenvalues and the order 1 Riesz means are related by the Legendre transform [29]. It is a small modification of this insight that will allow us to obtain the bound from Lemma 4.1 with $\gamma = 1$.

By Lemma 4.1 it, for any $k \in \mathbb{N}$, follows that

$$\begin{aligned} \sup_{\lambda \geq 0} \left(k\lambda - \sum_{i: \lambda_i \leq \lambda} (\lambda - \lambda_i(R)) \right) &\geq \sup_{\lambda \geq 0} \left(k\lambda - L_{1,n}^{\text{cl}} \lambda^{1+n/2} + \frac{3bL_{1,n-1}^{\text{cl}}}{8a_1} \lambda^{1+(n-1)/2} \right. \\ &\quad \left. - \frac{b^2 L_{1,n-2}^{\text{cl}}}{8\pi a_1^2} \lambda^{1+(n-2)/2} \right). \end{aligned} \quad (27)$$

The supremum on the left-hand side is achieved precisely at $\lambda = \lambda_k(R)$. Indeed, the function $f_k(\lambda) = k\lambda - \sum_{i: \lambda_i \leq \lambda} (\lambda - \lambda_i(R))$ is continuous, increasing for all λ for which $N(\lambda, R) < k$, and decreasing if $N(\lambda, R) > k$. Moreover, for λ such that $N(\lambda, R) = k$ we have that $f_k(\lambda) = \sum_{i=1}^k \lambda_i(R)$. Thus the left-hand side reduces to

$$\sup_{\lambda \geq 0} \left(k\lambda - \sum_{i: \lambda_i \leq \lambda} (\lambda - \lambda_i(R)) \right) = \sum_{i=1}^k \lambda_i(R).$$

On the other hand, maximising the right-hand side of the inequality is slightly more difficult and there may also be a question of uniqueness of the maximum. However, on this side we may choose any $\lambda \geq 0$ and still obtain a valid inequality.

Choosing λ to maximise $k\lambda - L_{1,n}^{\text{cl}} \lambda^{1+n/2}$, which corresponds to

$$\lambda = \left(\frac{k}{(\frac{n}{2} + 1)L_{1,n}^{\text{cl}}} \right)^{2/n} = 4\pi \Gamma\left(\frac{n}{2} + 1\right)^{2/n} k^{2/n},$$

ensures that the leading order term has the sharp constant (this follows from the equivalence, via the Legendre transform, of the Li–Yau inequality for the sum of eigenvalues and the Berezin inequality for the Riesz mean of order $\gamma = 1$, see [29]). With the above choice of λ we obtain from (27) the bound

$$\sum_{i=1}^k \lambda_i(R) \geq \frac{4\pi n \Gamma(\frac{n}{2} + 1)^{2/n}}{n+2} k^{1+2/n} + \frac{3\pi b \Gamma(\frac{n}{2} + 1)^{1+1/n}}{2a_1 \Gamma(\frac{n+3}{2})} k^{1+1/n} - \frac{b^2}{2a_1^2} k,$$

which completes the proof. \square

With the above bounds in hand, and almost step-by-step following the proof in Section 2.2, or the corresponding proof in [32], one obtains that R_λ^D, R_μ^N and \bar{R}_k^D are uniformly bounded as λ, μ or k goes to infinity. For the Riesz means, in both the Dirichlet case and the Neumann case, the proof is completely analogous to that in Section 2.2 by using the asymptotic expansions given on page 11.

For the eigenvalue averages we require an upper bound for $\frac{1}{\bar{a}_{1,k}k^{1/n}}$, which can be obtained as follows. Since \bar{R}_k^D is a minimiser, we have that

$$\frac{k\pi^2}{\bar{a}_{1,k}^2} \leq k\lambda_1(\bar{R}_k^D) \leq \sum_{i=1}^k \lambda_i(\bar{R}_k^D) \leq \sum_{i=1}^k \lambda_i(Q).$$

Inserting that, as $k \rightarrow \infty$,

$$\sum_{i=1}^k \lambda_i(Q) = \frac{4\pi n \Gamma(\frac{n}{2} + 1)^{2/n}}{n+2} k^{1+2/n} + \frac{2\pi \Gamma(\frac{n}{2} + 1)^{1+1/n}}{(n+1)\Gamma(\frac{n+1}{2})} |\partial Q| k^{1+1/n} + o(k^{1+1/n})$$

and rearranging implies the required bound.

The asymptotic expansions for the Riesz means of an arbitrary cuboid can be obtained by applying the Aizenman–Lieb identity to the asymptotic expansions of the counting functions. For the asymptotics of the eigenvalue averages, one can make use of the corresponding two-term expansions that we have for $\lambda_i(R)$ and calculate the asymptotics of the resulting sums (for instance using the Euler–Maclaurin formula).

In a similar manner as in the preceding section, one could for these problems also obtain estimates for the spectral stability, i.e. to what order in the respective parameters do the extremal eigenvalue means or averages approach those of the limiting domain Q . However, by finer analysis of the asymptotics, and not lifting the results for the counting function, it should be possible to obtain sharper estimates than what is obtained directly by the method outlined in the previous paragraph. This is due to the fact that in the above problems the erratic behaviour of the eigenvalues and counting function has in some sense been reduced.

It is possible to analyse the asymptotic behaviour of the extremal averages of the first k Neumann eigenvalues among unit measure cuboids by invoking Theorem 1.3. Indeed, by using that

$$\frac{1}{k} \sum_{i=0}^k \mu_i(Q) \leq \sup \left\{ \frac{1}{k} \sum_{i=0}^k \mu_i(R) : R = R_{a_1, \dots, a_n}, |R| = 1 \right\} \leq \frac{1}{k} \sum_{i=0}^k \mu_i^N$$

and Theorem 1.3, one obtains precise two-term asymptotics for the extremal averages, and finds that they agree with the corresponding asymptotics for Q . However, we have so far been unable to obtain an inequality which is sharp enough to conclude that the sequence of extremal cuboids for this problem remains uniformly bounded as $k \rightarrow \infty$. Thus our approach yields nothing about the geometric convergence.

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APPENDIX A. ONE-DIMENSIONAL BOUNDS

Lemma A.1. *For $\lambda \geq 0$ and $a > 0$ we have that*

$$\mathrm{Tr}(-\Delta_{(0,a)}^{\mathcal{D}} - \lambda)_-^{3/2} \leq aL_{3/2,1}^{cl}\lambda^2 - \frac{3b}{8}L_{3/2,0}^{cl}\lambda^{3/2} + \frac{b^2}{8\pi a}L_{3/2,-1}^{cl}\lambda,$$

for all $b \in [0, b_0]$, with $b_0 := \pi - \sqrt{\frac{6-8\pi+3\pi^2}{3}}$.

Lemma A.2. *For $\mu \geq 0$ and $a > 0$ we have that*

$$\mathrm{Tr}(-\Delta_{(0,a)}^{\mathcal{N}} - \mu)_-^{1/2} \geq aL_{1/2,1}^{cl}\mu + \left(1 - \frac{\pi}{4}\right)L_{1/2,0}^{cl}\mu^{1/2}.$$

Moreover, both constants are sharp.

Remark A.3. For our purposes the size of the coefficient of $\mu^{1/2}$ is of little importance as long as it is positive. Certain parts of the proof are simplified if one is not aiming for a sharp constant, but for completeness we show how to obtain the sharp bound.

Proof of Lemma A.1. Since $\lambda((0,a)) = \pi^2/a^2$ we know that $\mathrm{Tr}(-\Delta_{(0,a)}^{\mathcal{D}} - \lambda)_-^{3/2} = 0$ for $\lambda \leq \pi^2/a^2$. To get a bound for $\lambda > \pi^2/a^2$ we apply the following inequality which is due to Geisinger–Laptev–Weidl [16],

$$\mathrm{Tr}(-\Delta_I^{\mathcal{D}} - \lambda)_-^{\gamma} \leq L_{\gamma,1}^{cl} \int_I \left(\lambda - \frac{1}{4\delta(t)^2} \right)_+^{\gamma+1/2} dt,$$

valid for $\lambda \geq 0$ and $\gamma \geq 1$, where $I \subset \mathbb{R}$ and $\delta(t) = \mathrm{dist}(t, I^c)$. For $\lambda \geq 1/a^2$ this implies that

$$\begin{aligned} \mathrm{Tr}(-\Delta_{(0,a)}^{\mathcal{D}} - \lambda)_-^{3/2} &\leq 2L_{3/2,1}^{cl} \int_0^{a/2} \left(\lambda - \frac{1}{4t^2} \right)_+^2 dt \\ &= L_{3/2,1}^{cl} \left(a\lambda^2 - \frac{8}{3}\lambda^{3/2} + \frac{2}{a}\lambda - \frac{1}{3a^3} \right). \end{aligned} \quad (28)$$

We aim for a bound of the form $\mathrm{Tr}(-\Delta_{(0,a)}^{\mathcal{D}} - \lambda)_-^{3/2} \leq L_{3/2,1}^{cl}\lambda(\sqrt{a\lambda} - b/\sqrt{a})^2$, which holds for all $\lambda \geq 0$ and some $b > 0$. Note that this bound holds trivially for all $\lambda \leq \pi^2/a^2$, and thus we only need to choose b so that it is valid for all $\lambda > \pi^2/a^2$. Moreover, note that this bound, for $b < \pi$ and $\lambda > \pi^2/a^2$, is pointwise decreasing in b . Hence if we know the bound to hold for some b_0 then it holds for all $0 \leq b \leq b_0$.

Since we have an upper bound in terms of the polynomial in (28), it suffices to choose b so that, for all $\lambda > \pi^2/a^2$,

$$a\lambda^2 - \frac{8}{3}\lambda^{3/2} + \frac{2}{a}\lambda - \frac{1}{3a^3} \leq \lambda \left(\sqrt{a\lambda} - \frac{b}{\sqrt{a}} \right)^2 = a\lambda^2 - 2b\lambda^{3/2} + \frac{b^2}{a}\lambda,$$

Rearranging we see that this is equivalent to

$$\left(\frac{2}{a} - \frac{b^2}{a} \right) \lambda - \frac{1}{3a^3} \leq \left(\frac{8}{3} - 2b \right) \lambda^{3/2},$$

and thus we must choose $b < 4/3$. If this is true then, since $\lambda > \pi^2/a^2$,

$$\left(\frac{8}{3} - 2b \right) \lambda^{3/2} \geq \left(\frac{8}{3} - 2b \right) \frac{\pi}{a} \lambda.$$

Thus it is sufficient to choose b satisfying

$$\left(\frac{2}{a} - \frac{b^2}{a} \right) \lambda - \frac{1}{3a^3} \leq \left(\frac{8}{3} - 2b \right) \frac{\pi}{a} \lambda.$$

Or equivalently so that

$$\left(2 - b^2 - \frac{8\pi}{3} + 2b\pi \right) \lambda \leq \frac{1}{3a^2},$$

but this holds for all $\lambda > \pi^2/a^2$ if and only if the left-hand side is non-positive. Finding the roots of the quadratic expression in b and taking into account the requirement $b < 4/3 < \pi$, we find that we may choose any $b \leq b_0 = \pi - \sqrt{\frac{6-8\pi+3\pi^2}{3}}$.

Thus for all $0 \leq b \leq b_0$ and $\lambda \geq 0$ we have the three-term bound

$$\begin{aligned} \text{Tr}(-\Delta_{(0,a)}^{\mathcal{D}} - \lambda)_-^{3/2} &\leq L_{3/2,1}^{\text{cl}} \lambda (\sqrt{a\lambda} - b/\sqrt{a})^2 \\ &= aL_{3/2,1}^{\text{cl}} \lambda^2 - \frac{3b}{8} L_{3/2,0}^{\text{cl}} \lambda^{3/2} + \frac{b^2}{8\pi a} L_{3/2,-1}^{\text{cl}} \lambda, \end{aligned}$$

which is the claimed bound. \square

Proof of Lemma A.2. That the leading constant is sharp follows from the corresponding Weyl asymptotics (c.f. page 11). As we also have equality for $\mu = \mu_1((0, a)) = \pi^2/a^2$, the coefficient of $\mu^{1/2}$ is the largest possible.

By scaling it is clear that the bound is equivalent to that, for $r \geq 0$,

$$\sum_{k=0}^{\infty} (r^2 - k^2)_+^{1/2} \geq \frac{\pi}{4} r^2 + \left(1 - \frac{\pi}{4} \right) r. \quad (29)$$

We begin by observing that between integer values of r the sum is concave as a function of r , since the polynomial $\frac{\pi}{4} r^2 + \left(1 - \frac{\pi}{4} \right) r$ is convex it is thus sufficient to establish that the inequality holds for integer values of r .

To this end, for $r = m \in \mathbb{N}$, we rewrite our sum:

$$\begin{aligned} \sum_{k=0}^{m-1} \sqrt{m^2 - k^2} &= \sum_{k=0}^{m-1} \sqrt{m^2 - k^2} - \sum_{k=0}^{m-1} \frac{\sqrt{m^2 - k^2} - \sqrt{m^2 - (k+1)^2}}{2} + \frac{m}{2} \\ &= m^2 \left(\frac{1}{m} \sum_{k=0}^{m-1} \sqrt{1 - \left(\frac{k}{m}\right)^2} - \sum_{k=0}^{m-1} \frac{\sqrt{1 - \left(\frac{k}{m}\right)^2} - \sqrt{1 - \left(\frac{k+1}{m}\right)^2}}{2m} \right) + \frac{m}{2}. \end{aligned}$$

We now recognise the expression in the parenthesis as the approximation of the integral $\int_0^1 \sqrt{1-t^2} dt$ using the trapezoid method with $[0, 1]$ divided into m equal intervals. Thus we find that

$$\begin{aligned} \sum_{k=0}^{m-1} \sqrt{m^2 - k^2} &= m^2 \left(\int_0^1 \sqrt{1-t^2} dt - E_T(m) \right) + \frac{m}{2} \\ &= \frac{\pi}{4} m^2 + \frac{m}{2} - m^2 E_T(m), \end{aligned}$$

where $E_T(m)$ denotes the error in the trapezoid approximation with m equal subintervals. To complete the proof we need to show that $mE_T(m) \leq \frac{\pi}{4} - \frac{1}{2}$.

As $\sqrt{1-t^2}$ is concave and decreasing on $[0, 1]$, $E_T(m)$ is positive. The error of the m -interval trapezoid approximation of an integral $\int_a^b f(t) dt$ is bounded from above by

$$\frac{(b-a)^3}{12m^2} \sup_{t \in [a,b]} |f''(t)|.$$

But as the function of interest here has unbounded second derivative at $t = 1$ applying this bound directly is not possible. However, we can use this on the interval $[0, k'/m]$ for some integer $k' \in \{0, \dots, m-1\}$. On the remaining interval $[k'/m, 1]$ we estimate the error simply by the difference between the trapezoid approximation and the upper Riemann sum, i.e. we add the area of the triangles completing the trapezoids into rectangles.

This yields the estimate

$$\begin{aligned} E_T(m) &\leq \inf_{k' \in \{0, \dots, m-1\}} \left(\frac{(k'/m)^3}{12(k')^2(1 - (k'/m)^2)^{3/2}} + \sum_{k=k'}^{m-1} \frac{\sqrt{1 - \left(\frac{k}{m}\right)^2} - \sqrt{1 - \left(\frac{k+1}{m}\right)^2}}{2m} \right) \\ &= \inf_{k' \in \{0, \dots, m-1\}} \left(\frac{k'}{12(m^2 - (k')^2)^{3/2}} + \frac{\sqrt{m^2 - (k')^2}}{2m^2} \right) \\ &< \left(\frac{m - 2\sqrt{m}/5}{12(m^2 - (m - 2\sqrt{m}/5)^2)^{3/2}} + \frac{\sqrt{m^2 - (m - 2\sqrt{m}/5 - 1)^2}}{2m^2} \right), \end{aligned}$$

where in the last step we set $k' = \lfloor m - 2\sqrt{m}/5 \rfloor$ and estimate this from above and below. Define, for $\eta \geq 1$,

$$g(\eta) = \eta^2 \left(\frac{\eta^2 - 2\eta/5}{12(\eta^4 - (\eta^2 - 2\eta/5)^2)^{3/2}} + \frac{\sqrt{\eta^4 - (\eta^2 - 2\eta/5 - 1)^2}}{2\eta^4} \right).$$

If we can show that $g(\eta) \leq \frac{\pi}{4} - \frac{1}{2}$ then we are done. Unfortunately this is not true, for small m our bound for the error is not sharp enough. However, for the first couple of integers m it is easy to check by hand that (29) holds. It is clear that $g(\eta) \rightarrow 0$ as $\eta \rightarrow \infty$, and by differentiating g it is possible to see that g is strictly decreasing for $\eta \geq 2$ (g' can be written as quotient with positive denominator and all positive terms in the numerator can be majorised by the higher order negative terms). Furthermore, one can check that

$$g(\sqrt{28}) < g(5 + 1/5) = \frac{1}{20} + \frac{5\sqrt{3927}}{1352} < \frac{\pi}{4} - \frac{1}{2}.$$

Thus the inequality (29) is true for all $r \geq 28$, the remaining cases can be checked by hand or using a computer. If one settles for a non-sharp coefficient of $\mu^{1/2}$, then the number of terms to check by hand can be reduced to five. \square

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